POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 38th cycle

PNRR_352 Research Field: MODELLING OF THE PHYSICAL AND CHEMICAL ABSORPTION OF ACID GASES IN WATER-FREE SOLVENTS

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	The research project focuses on the development of a green solvent for the process of CO_2 capture from flue gas streams to reduce greenhouse gas emissions to the atmosphere. Decarbonization and reduction of emissions are relevant topics of the considered thematic area ("Rivoluzione verde e transizione ecologica") and, in general, of PNRR.In particular, the aim of the research is the study of an absorption process based on the use of innovative physical and chemical solvents with low environmental impact for acid gas purification to be applied in power production systems.For reducing the CO_2 content in flue gas streams before their emission in the atmosphere, chemical absorption is the most suitable technology, with MonoEthanolAmine (MEA) aqueous solution being the traditional solvent used for this aim. Aqueous amine solutions are also employed for acid gas removal to treat gaseous streams for accomplishing product specifications. However, they are characterized by high energy requirement, in particular in the regeneration section, corrosion and toxicity. All these issues make the overall absorption system economically and environmentally uncompetitive.With the aim of employing a low impact technology for removal of CO_2, new generation solvents are under study. Recently, research has focused on water

	-lean or water-free solvents, with a reduction of or the absence of the water content and the possible substitution of the amine with another reacting species. The advantage is the enhancement of the physical absorption capabilities of the solvent without affecting too significantly the chemical properties and the reduction of the energy requirements in the regeneration section, the most energy demanding part of the plant, due to the parasitic heat losses for water vaporization. Moreover, some species composing the innovative solvent can be produced from renewable sources, thus further reducing the environmental impact.Few studies on this topic have been performed until now and there is a lack of experimental data in the literature regarding this type of innovative (green) solvents. Therefore, the main objectives of the research activity are: • set-up of the apparatus for the collection of experimental data needed for the modeling of the system of interest; • experimental measurements (*i.e.*, vapor-liquid equilibrium and liquid-liquid equilibrium of the solvent mixture, solubility of CO_2 in the solvent, kinetics of CO_2 absorption); • thermodynamic and mass transfer modeling; • simulation of the process of absorption and regeneration; • application to the treatment of a flue gas stream from power plant.
Methods and techniques that will be developed and used to carry out the research	The research activity will involve: • an experimental activity aimed at filling the gap regarding phase equilibrium and kinetic data for the solvent mixture of interest; • a modelling activity for selecting a proper thermodynamic model and a mass transfer model to describe the mixtures of interest in a reliable way; • a simulation activity aimed at representing the CO_2

	capture system composed of an absorption section and a solvent regeneration section; • an evaluation activity for determining the performances of the proposed solvent for application to the treatment of a flue gas stream from power plant. The experimental activity will involve the use of an apparatus already available in the *Process Thermodynamics laboratory* (PT lab) of Politecnico di Milano for the collection of Vapor-Liquid Equilibrium and Liquid-Liquid Equilibrium data and the use of an apparatus for the determination of the kinetics of the system which will be installed in Eni S.p.A. for the duration of this research. During this activity the most suitable measurement procedures for the collection of experimental data will be defined.The modelling and simulation activities will be carried out at Politecnico di Milano in collaboration with Eni S.p.A.. The modelling activity will include the calibration of thermodynamic models by regression of their parameters, exploiting both the experimental data available in the literature, if available, and those collected during the experimental campaign in this research, and the choice of a method for the description of mass transfer (with reaction). The simulation activity will be based on commercial process simulation software, whose database will be integrated with the addition of the compounds present in the innovative solvent studied, if not already available, and which will be linked to external subroutines if required. For the activity related to the evaluation of the performances of the process applied to the treatment of a flue gas stream from power plant, a sensitivity analysis on the main process parameters will be performed to determine the best process scheme, with minimization of the energy requirements.
Educational objectives	From an educational point of view, the planned research activity is expected to improve the capabilities of the PhD candidate in providing cutting-edge and sustainable solutions. By using the acquired knowledge, in particular related to chemical, physical, mathematical and

	engineering topics, the PhD graduate will be able to qualitatively and quantitatively describe chemical-physical transformations, and, on this basis, to design processes able to meet the needs of society.
Job opportunities	The PhD graduate will have the expertise for starting a professional career in national and multinational companies related to process engineering (*i.e.*, in the Oil&Gas field, in the basic chemistry field), with recognition of the experience gained during the PhD.
Composition of the research group	1 Full Professors 1 Associated Professors 2 Assistant Professors 3 PhD Students
Name of the research directors	Prof. L.A. Pellegrini /Ing. G. Filippini (Eni)

Contacts
laura.pellegrini@polimi.it gasp.chem.polimi.it/

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	Eni S.p.A.
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	The project promotes international collaborations with high-level research centers abroad focusing on Carbon Capture & Storage, in particular as for the collection of experimental data of interest for the innovative solvent in the institution abroad to be used for thermodynamic and mass transfer modeling and process simulation in Italy.
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Confidentiality: since this is a thematic scholarship, the management of Confidential Information,

Results and their publication is subordinate to the restrictions agreed upon with the funding company. Upon acceptance of the scholarship, the beneficiary must sign a specific commitment.

Individual budget for research (during the 3 years): about 5.400 euro

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial of for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.